



## Texture in the Post-Perovskite Phase: Towards an Understanding of Anisotropy in the D''

— Lowell Miyagi

### Texture in the Post-Perovskite Phase: Towards an Understanding of Anisotropy in the D''

Since the discovery of the phase transition in  $\text{MgSiO}_3$  from a perovskite to post-perovskite (pPv) structure at 127GPa and 2500K (Murakami et al 2004), there has been considerable interest in the mechanical properties of the pPv structure.  $\text{MgSiO}_3$  pPv may be a major constituent of the D'' layer which lies above the core-mantle boundary (e.g. Murakami et al 2004). The D'' is a region characterized by a seismic discontinuity that also exhibits significant lateral heterogeneity and seismic anisotropy (e.g. Panning and Romanowicz 2004). First-principles calculations using density functional theory and available experiments suggest that  $\text{MgSiO}_3$  pPv exhibits strong elastic anisotropy (e.g. Murakami et al., 2004, Oganov and Ono, 2004).

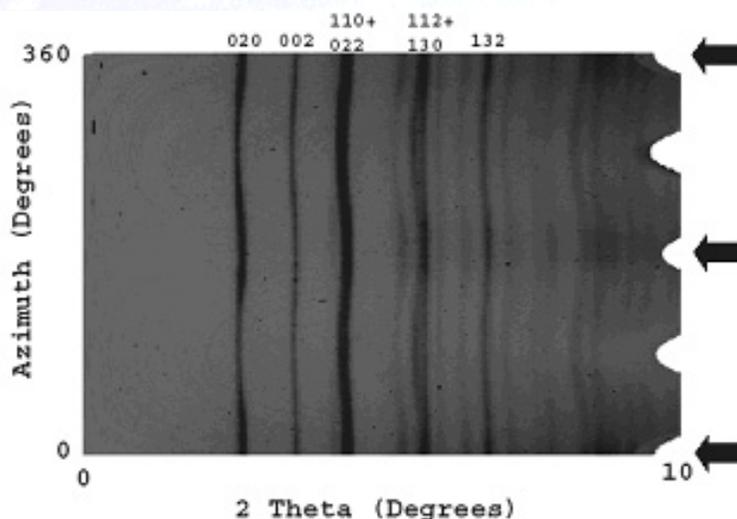
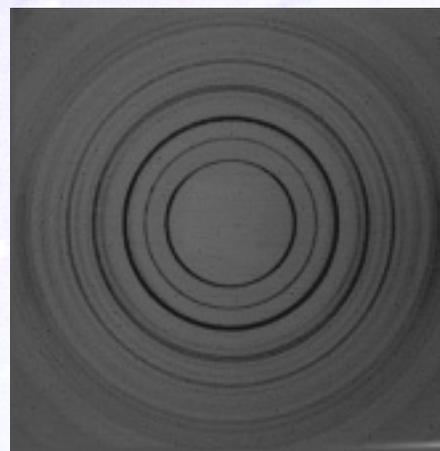


Figure 1. a) Raw diffraction image of  $\text{CaIrO}_3$  at 2.5 GPa (Miyagi et al 2006). b) “Unrolled” diffraction pattern of image in part a). Lattice strains as a result of differential stresses are visible as variation in peak positions with azimuth. Intensity variations with azimuth are also visible and are indicative of texture. Major peaks are labeled and the compression direction is indicated by block arrows.

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One mechanism that can generate seismic anisotropy is the development of lattice preferred orientation (LPO) or texture, during plastic deformation of aggregates composed of anisotropic minerals. Radial diffraction patterns obtained *in-situ* during deformation experiments with diamond anvil cells (DAC) and the multi-anvil press have been used successfully to observe texture changes and infer active slip-systems in a variety of deep earth relevant materials (e.g. Wenk et al 2006). In radial diffraction images, variations in lattice spacings with respect to the compression direction are due to elastic strains imposed by the deformation device. These manifest as sinusoidal variations in peak positions with azimuth. Preferred orientation resulting from plastic deformation appears as systematic intensity variations along Debye rings. If lattice planes in a sample are predominantly oriented in a particular direction, then more intense diffraction will be observed in that direction (Fig. 1). By deconvoluting this information the full orientation distribution (OD) can be determined.

Since  $\text{MgSiO}_3$  pPv is unquenchable to ambient conditions, deformation studies are difficult and limited. One major limitation is that current technology does not allow

for *in-situ* radial diffraction and simultaneous deformation at high-temperatures and pressures in the stability field of  $\text{MgSiO}_3$  pPv. For  $\text{MgSiO}_3$  pPv, this makes it virtually impossible to investigate the possibility of high-temperature slip-systems which may have a significant effect on texturing. As a result of this limitation the investigation of analog materials is of interest.  $\text{CaIrO}_3$  pPv is a potentially useful low pressure analog and allows for deformation in the multi-anvil press. The multi-anvil press has a limited pressure range when compared to the DAC, however, it provides better control of stress state as well as the ability to deform at high temperatures.

A recent study by Miyagi et al (2006) deformed  $\text{CaIrO}_3$  pPv in the D-DIA multi-anvil press at a variety of pressures and temperatures up to 5 GPa and 1500K. Using *in-situ* radial diffraction and the Rietveld method to extract quantitative texture information, this study found that during compression lattice planes oriented with the (010) planes perpendicular to the compression axis. In the case of axial compression, cylindrical symmetry about the compression

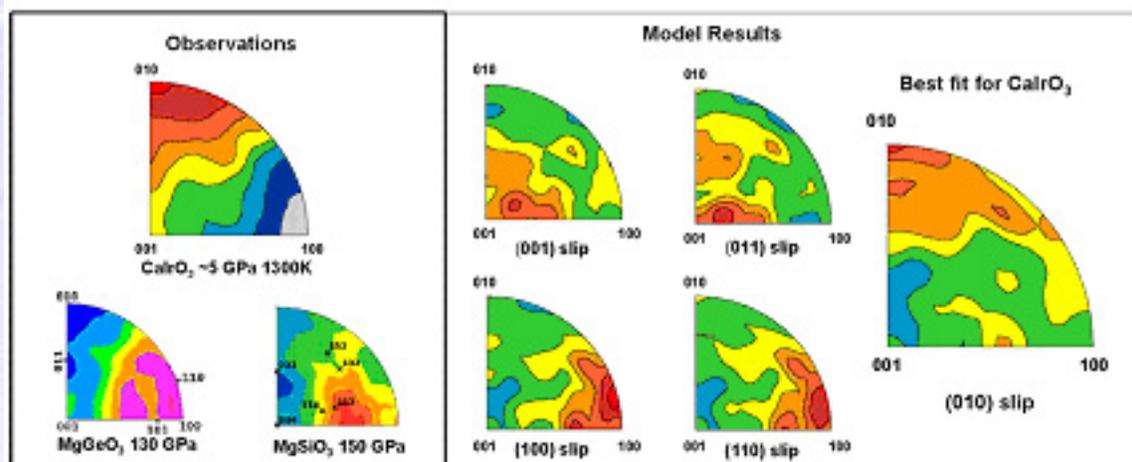


Figure 2. Inverse pole figures of experimental data on pPv structures and results from polycrystal plasticity models. Warmer colors indicate a high probability of finding a slip plane oriented perpendicular to compression while cooler colors indicate a reduced probability. (left side) A comparison of experimental inverse pole figures summarizing texture data for  $\text{CaIrO}_3$  pPv (Miyagi et al 2006),  $\text{MgGeO}_3$  pPv (Merkel et al 2006) and  $\text{MgSiO}_3$  pPv (Merkel et al 2007). (right) Inverse pole figures of polycrystal plasticity modeling results for models favoring dominant slip on (001), (011), (100), (110), and (010). The room-temperature data for  $\text{MgGeO}_3$  pPv and  $\text{MgSiO}_3$  pPv are best explained by dominant slip on (100) and (110) or some combination of the two systems (Merkel et al 2006, 2007).  $\text{CaIrO}_3$  pPv, in contrast is best explained by dominant slip on the (010) plane (Miyagi et al 2006).

axis can be assumed and textures can be compactly represented with an inverse pole figure (IPF). IPFs show the relationship between poles (normals) to the lattice planes of crystallites in the sample to the compression direction (Fig 2). The texture obtained by Miyagi et al (2006) was consistent for all temperatures and pressures accessed during this experiment, indicating that there is little effect of temperature on the slip systems of  $\text{CaIrO}_3$  pPv.

By comparing synthetic textures generated with polycrystal plasticity models to experimental textures, active slip systems can be inferred for a given set of deformation conditions. The development of textures depends on the deformation geometry and the relative activities of various slip systems. Starting with an initially random distribution of crystallite orientations and assuming deformation by intracrystalline slip, an incremental deformation path can be applied. As deformation proceeds, crystals deform and rotate to generate preferred orientation. By applying different critical resolved shear stresses to slip systems, one slip system will be favored over another, resulting in different textures for different slip system combinations. By determining which simulated texture most closely resembles the experimental texture, it can be inferred which slip systems are active under the experimental conditions.

Polycrystal plasticity models indicate that preferential (010)[100] slip produces a distinct maximum around (010) that closely resembles the experimental textures for  $\text{CaIrO}_3$  pPv (Fig 2). It is therefore likely that (010)[100] is the dominant slip system at all conditions of these experiments (Miyagi et al 2006). This result is consistent with a previous transmission electron microscopy (TEM) study of dislocation microstructures generated during synthesis of  $\text{CaIrO}_3$  pPv. This study identified slips with a Burgers vector  $b = [100]$  and  $b = [u0w]$  and suggested that (010) is the likely slip plane (Miyajima et al 2006). A TEM study of recovered samples from a shear deformation experiment on  $\text{CaIrO}_3$  pPv also observed the [100](010) slip system (Yamazaki et al 2006). Based on structural considerations it had been suggested that the pPv structure would slip on the (010) plane, consistent with the layered structure (e.g. Murakami et al 2004; Oganov and Ono 2004).

Results for  $\text{CaIrO}_3$  pPv are in contrast with previous room-temperature texture measurements on  $\text{MgGeO}_3$  pPv (Merkel et al 2006) and  $\text{MgSiO}_3$  pPv (Merkel et al 2007) in the DAC (Fig 2). Here a maximum near (100) and a distinct minimum of (010) was observed and inter-

preted as evidence for slip on (100) and (110) planes in agreement with first principles calculations (Oganov et al 2005). Experimental results on  $\text{Mn}_2\text{O}_3$  post-perovskite observed both of these textures (Santillán et al 2006). Prior to annealing it was observed that the (010) lattice planes were oriented perpendicular to compression. After annealing it was noted that lattice preferred orientation changed to the (100) and (110) planes perpendicular to compression.

One explanation for this contrasting behavior is that the interatomic potential between the layers in the pPv structure and the interlayer cations is different for  $\text{CaIrO}_3$  and  $\text{MgSiO}_3$  pPv.  $\text{CaIrO}_3$  behaves as a sheet structure and slips along these layers.  $\text{MgSiO}_3$  on the other hand has stronger coupling across the layers and slip does not occur along the layered structure. Similar differences in slip systems are well known for other structures. This explanation, however, does not necessarily explain why both textures were observed in  $\text{Mn}_2\text{O}_3$ , and clearly more work needs to be done both on analog materials and  $\text{MgSiO}_3$  pPv in order to elucidate our understanding of the systematic rheology of pPv structures and provide a better understanding of the behavior of  $\text{MgSiO}_3$  pPv in the deep earth.

## Selected References

1. M. Murakami, K. Hirose, K. Kawamura, N. Sata, Y. Ohishi (2004), Post-Perovskite Phase Transition in  $\text{MgSiO}_3$ , *Science* **304**, 855.
2. A. R. Oganov, S. Ono (2004), Theoretical and experimental evidence for a post-perovskite phase of  $\text{MgSiO}_3$  in Earth's D'' layer, *Nature* **430**, 445.
3. M. Panning, B. Romanowicz (2004), Inferences on Flow at the Base of Earth's Mantle Based on Seismic Anisotropy, *Science* **303**, 351.
4. H.-R. Wenk, I. Lonardelli, S. Merkel, L. Miyagi, J. Pehl, S. Speziale, C. E. Tommaseo (2006), Deformation textures produced in diamond anvil experiments, analysed in radial diffraction geometry, *J. Phys. Cond. Matt.*, **18** (25), S933.

5. L. Miyagi, N. Nishiyama, Y. Wang, A. Kubo, D. V. West, R. J. Cava, T. S. Duffy, H.-R. Wenk (2006), Deformation of the  $\text{CaIrO}_3$  post-perovskite phase to 5 GPa and 1300 K in the multi-anvil press, *EOS Trans. AGU Fall Meet. Suppl.* **87**, Abstract MR11B-0128.
6. N. Miyajima, K. Ohgushi, M. Ichihara, T. Yagi (2006), Crystal morphology and dislocation microstructures of  $\text{CaIrO}_3$ : A TEM study of an analogue of the  $\text{MgSiO}_3$  post-perovskite phase, *GRL* **33**, L12302, doi:10.1029/2005GL025001.
7. D. Yamazaki, T. Yoshino, H. Ohfuji, J.-I. Ando, A. Yoneda (2006), Origin of seismic anisotropy in the D' layer inferred from shear deformation experiments on post-perovskite phase, *EPSL* **252**, 372.
8. A. R. Oganov, R. Martoňák, A. Laio, P. Raiteri, M. Parrinello (2005), Anisotropy of Earth's D' layer and stacking faults in the  $\text{MgSiO}_3$  post-perovskite phase, *Nature* **438**, 1142.
9. S. Merkel, A. Kubo, L. Miyagi, S. Speziale, T. S. Duffy, H.-K. Mao, H.-R. Wenk (2006), Plastic deformation of  $\text{MgGeO}_3$  post-perovskite at lower mantle pressures, *Science* **311**, 5761.
10. S. Merkel, A. K. McNamara, A. Kubo, S. Speziale, L. Miyagi, Y. Meng, T. S. Duffy, H.-R. Wenk (2007), Deformation of  $(\text{Mg,Fe})\text{SiO}_3$  post-perovskite and D' Anisotropy, *Science* in press.
11. J. Santillán, S. H. Shim, G. Shen, V. B. Prakapenka (2006), High-pressure phase transition in  $\text{Mn}_2\text{O}_3$ : Application for the crystal structure and preferred orientation of the  $\text{CaIrO}_3$  type, *GRL* **33**, L15307, doi:10.1029/2006GL026423.

## Acknowledgements

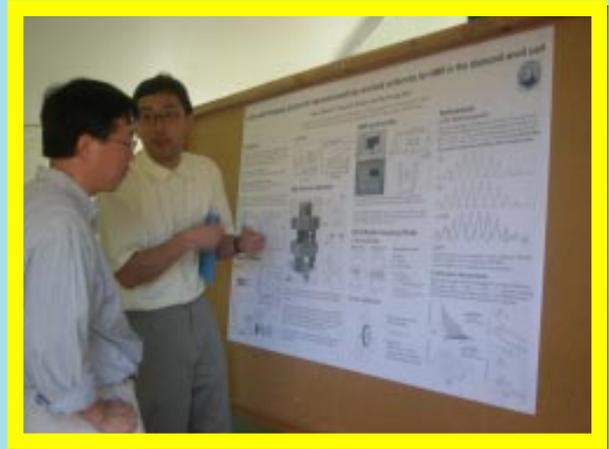
This article is derived from a series of collaborations between UC Berkeley, Princeton, and scientists at the Advanced Photon Source (APS). Experiments were conducted at HP-CAT and GSECARS sectors of the APS. These facilities are partially funded by COMPRES. Additional support was received from CDAC.

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## Thank you to Jiuhua Chen

— Bob Liebermann

This issue of the COMPRES Newsletter is the last one being edited by Jiuhua Chen, Research Professor in the Mineral Physics Institute of Stony Brook University. In September 2007, Jiuhua will be leaving Stony Brook to take up a position as an Associate Professor in the Department of Mechanical and Materials Engineering of Florida International University. At FIU, he will also have an affiliation with the Center for the Study of Matter at Extreme Conditions directed by Surendra Saxena.



On behalf of the COMPRES Executive Committee and the entire community, I would like to thank Jiuhua for creating the concept of the regular Newsletter and for serving as its editor for the first 15 issues from November 2002 to August 2007.

# COMPRES Funding Renewed

The proposal requesting renewed funding for COMPRES [Proposal EAR-0649658], "*COMPRES: Com-munity Facilities and Infra-structure Development for High-Pressure Mineral Physics and Geosciences*" has been reviewed by the Instrumentation & Facilities Program in the Division of Earth Sciences (EAR/IF).

The NSF has approved renewal of the Cooperative Agreement via which COMPRES will be supported for another 5-year period from May 1, 2007 to April 30, 2012. On behalf of the Executive Committee and the Standing Committees, I would like to thank all members of the COMPRES community for your contributions to the renewal proposal in August 2006 and the Site Visit in November 2006, which formed the basis for the case for renewing funding for COMPRES.

In the context of fiscal realities in Washington, and in the NSF and within EAR, our community is fortunate in securing this funding, even though it is less than the amount we requested in the August 2006 proposal.

Funding this fiscal year [May 1, 2007 to April 30, 2008] will be recommended at \$2,100,000. The level of continued NSF support will be negotiated with COMPRES annually, with continuation of NSF support dependent upon an annual review of accomplishments, availability of funds, and scientific progress. Contingent on the availability of funds and the scientific progress of the project, NSF expects to continue support of COMPRES at approximately the following levels:

\$2,200,000	FY 2008
\$2,300,000	FY 2009
\$2,400,000	FY 2010
\$2,500,000	FY 2011

## Thanks to Harry Green for Superior Leadership

— Bob Liebermann

On behalf of the entire COMPRES community, I would like to thank Harry Green for his leadership of COMPRES as the Chair of the Executive Committee for the past three years [2004-2007].

Harry is a distinguished scientist, and experienced administrator, and an articulate spokesperson, and he has given generously of his time and energy in leading our organization through a very formative period of our existence, including the 1 1/2 year process leading to the renewal of the Cooperative Agreement with the NSF for another 5 years.

COMPRES appreciates and recognizes the very important contributions that Harry has made and hopes that he will continue to remain engaged in our activities.



*At the Lake Morey meeting, Bob Liebermann presented Harry with a framed copy of the COMPRES poster [which not incidentally includes one of Harry's favorite diagrams about earthquakes in downgoing slabs in subduction zones].*

# MESSAGE TO THE COMPRES COMMUNITY FROM HARRY GREEN

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**To the COMPRES community:**

**Dear Colleagues:**

I write to you with two sets of very good news.

Firstly, the negotiations with NSF are now complete and I am delighted to inform you that COMPRES has been renewed for another 5 years. Due to severe budget restrictions at the Foundation, our budget could not be augmented for this first year. Nevertheless, it will grow modestly but steadily over the coming five years, budget realities permitting. One of the most rewarding aspects of the entire renewal review process has been the constant theme of congratulatory comments concerning the success of the first 5 years of COMPRES that we have received from within the Foundation and, most importantly, from a wide range of prominent members of other subgroups within the solid earth sciences. Thanks to your hard work, the transformation of our community from competitive mode to collaborative mode centered around the DOE beamline facilities has been achieved in a remarkably short time. I have heard numerous times from many colleagues that they are amazed by (and jealous of) how quickly our community has come together to work for support of the instrumentation and facilities needed by the community, including such things as communal sample assembly development, T and P calibration efforts, as well as development and benchmarking of new apparatus that take us to ever higher pressures, both for static and dynamic experiments. What impresses these colleagues most is that in doing so we have achieved a much stronger sense of community and common purpose while retaining our competitive spirit when it comes to what science individuals choose to push forward. Those of us serving on the COMPRES standing committees thank you all for your participation in this transformation and look for-

ward to many of you taking your turns participating in these important leadership positions.

Secondly, I am equally pleased to tell you that Bob Liebermann has agreed to another 5-year term as President of COMPRES. Throughout the critical last few years leading up to our renewal, it has been Bob who has been the glue that has held all of the pieces together and the memory of what needs to be done when. As Chair of the Executive Committee during these last 3 years, I have benefited immensely from Bob's competence, perseverance, and constant up-beat attitude and I know that my successor, to be chosen at this year's meeting at Lake Morey, VT, will benefit similarly. Our Consortium is in excellent hands and I look forward to another 5 years of growth and success for COMPRES.

I would also like to take the opportunity at this time to thank all of those who have served with me on the Executive Committee and equally those on the Facilities and Infrastructure Development Committees (listed below). Without exception, the members of these committees have given freely of their time and accepted the significant responsibilities thrust upon them. For an all-volunteer organization, we have been blessed with outstanding individuals who have stepped forward and worked hard for the benefit of all. I urge all of our membership to seriously consider accepting to serve when asked and to proactively seek such service if not asked. The broader the participation, the stronger will be COMPRES.

Harry  
Chair, COMPRES Executive Committee  
2003-2007

# President's Message

—**Bob Liebermann**

We are proud of the awards and honors recently bestowed on members of the COMPRES community. These include:

The following students received Outstanding Student Paper Awards at the 2006 Fall AGU Meeting from the Mineral and Rock Physics Focus Group:

- Gaurav Bhatnagar, Rice University, *Quantifying methane hydrate distribution in worldwide sediments: Comparison between observations and numerical simulations.*
- Liliana Boncalves-Ferreira, University of Cambridge, *Influence of defects on the twin wall structure of perovskite from molecular dynamics.*
- Kelly Havens, University of California Los Angeles, *High pressure electrochemical behavior of AgI.*
- Ran Holtzman, University of California Berkeley, *The strength of hydrate-bearing sediments: A grain-scale approach.*
- Hauke Marquardt, GeoForschungsZentrum Potsdam, *A systematic study on the thermal transport properties of natural and synthetic garnets.*
- Lowell Miyagi, University of California Berkeley, *Deformation of the  $\text{CaIrO}_3$  Post-perovskite phase to 5 GPa and 1300K in the multi-anvil press.*
- Antonio Piazzoni, Munich University, *Linking mineral physics and geodynamic mantle models.*

At the 2006 Fall Meeting of the AGU, Roberta Rudnick of the University of Maryland received the N. L. Bowen Award, which recognizes outstanding contributions to volcanology, geochemistry, or petrology.

The MSA recently announced its list of Distinguished Lecturers for 2006-2007. It was a pleasure to see the name of Steven D. Jacobsen from Northwestern University on this list and we send our congratulations to him for this recognition.

We were very pleased to learn that Russell Hemley has been selected to become the Director of the Geophysical Laboratory of the Carnegie Institution of Washington, effective July 1, 2007. We send our congratulations and best wishes to Rus on this honor and new leadership responsibility.

These distinctions, in addition to recognizing their significant achievements and contributions, brings honor and visibility to the community of mineral and rock physicists throughout the world.

On 4-5 January, I attended a meeting of the Science & Technology Steering Committee of the Brookhaven Science Associates at the Brookhaven National Laboratory. One of the principal agenda items was a presentation by Chi-Chang Kao (Chair of the NSLS) on the new five-year plan for NSLS-I and strategies for planning for the transition from NSLS-I to NSLS-II in 2013-14.

On January 26-28, I attended a COMPRES sponsored a "Workshop on the Current Status and Prospects for Establishing Precise and Accurate Pressure Scales at High Temperatures." This Workshop was convened by Alex Goncharov, Kurt Leinenweber, Tom Duffy, Rus Hemley, and Yingwei Fei and included more than 50 attendees from around the world.

From March 21 to April 1, I was in France for two events:

Visiting the laboratories at the Institut de Minéralogie et de Physique des Milieux Condensés in their new location at Boucicaut in southwest Paris on March 22-23. I gave a seminar on « Indoor Seismology » and discussed research projects with Guillaume Fiquet, James (Jimi) Badro, François Guyot, Frederic Decremps, Stefan Klotz and Michel Gauthier.

Attend the First EuroMinSci Conference in La Colle-sur-Loup near Nice in the south of France from March 26-29. This conference was convened by Bjorn Winkler of Universität Frankfurt and brought together faculty, staff and students from many countries in Europe who are engaged in the new European Mineral Sciences initiative, a 4-year collaborative research program supported by the European Collaborative Research Scheme [EUROCORES] of the European Science Foundation [ESF]. I gave the opening keynote talk on "Outdoor vs Indoor Geophysics." Other keynoters included H-k. (Dave) Mao of the Carnegie Institution of Washington.

# President's Message (cont'd)

I attended the semi-annual meeting of the CARS Board of Governors at the APS on April 13. Featured were presentations by GSECARS, which included examples of the collaboration of COMPRES and GSECARS in high-pressure mineral physics.

While at the APS, I had the opportunity to receive updates on several projects supported by COMPRES, including:

Johnson noise thermometry—Yanbin Wang, Mark Rivers and Ivan Getting. They have recently engaged a new postdoc, Takeshi Sanehira, to work on this project.

CO<sub>2</sub> Laser-heating system for DAC—Alexei Kuznetsov, Vitali Prakapenka and Guoyin Shen.

Brillouin spectrometer on 13 BM beamline—Jay Bass and Vitali Prakapenka.

Gas-loading system for DACS—Mark Rivers

Nuclear resonant inelastic scattering on Sec 3—Wolfgang Sturhahn.

D-DIA 30 apparatus—Yanbin Wang.

On April 19, I was at Delaware State University in Dover to help honor Gabriel Gwanmesia, who was recognized

for his research and educational achievements by an Innovative Technologies Breakfast sponsored by the Central Delaware Economic Development Council and the Delaware Economic Development Office, and Delaware State University.

On April 25, the Executive Committee of COMPRES visited NSF Headquarters to meet with Program Directors of the Division of Earth Sciences and the Department of Energy to discuss the current status of funding and future strategic initiatives for COMPRES.

On 8-13 May 2007, the High Pressure Mineral Physics Seminar-7 was held in Matsushima, Japan. Eiji Ohtani of Tohoku University in Sendai and his colleagues organized and executed a very successful meeting, both on a scientific and social level. Michael Brown of the University of Washington and Yanbin Wang of the University of Chicago served as the US conveners and Denis Andrault of Université Blaise Pascal in Clermont-Ferrand and David Rubie of the Bayerisches Geoinstitut served as the European conveners.

President's Message

## HPMP 2007 Matsushima, Japan



*Oral Presentations*



*Poster Session*



*Excursion*

# President's Message (cont'd)

As you may recall, this Seminar was the 7th in a series which dates back to 1976, when it was supported by the US-Japan cooperative program of the NSF International Program office. Although it is a continuation of that tradition, it has taken on a new flavor in the past two occurrences, the 2002 Seminar in Verbania, Italy, and the 2007 Seminar in Matsushima, Japan. It is now truly international, with strong contingents from Europe, Japan and the U. S., as well as attendees from Taiwan, China, and Canada.

The 2007 meeting was attended by more than 140 people, including 31 from European countries and 91 from the host country Japan. The U. S. was represented by 23 scientists from academic institutions and national laboratories. Although there were no graduate students in the U. S. contingent, there were 10 young faculty/staff persons, many of whom had never been to Japan. Of these young scientists, 4 were women. COMPRES received \$35,000 in special fund from the Office of International Science Exchanges and the Division of Earth Sciences at NSF to provide partial travel support for the US contingent.

The attendees have expressed a strong desire to have the next Seminar in 2012 in the U. S., and we in COMPRES have issued an "Olympic-style" invitation to all. We are already working to identify conveners for this Seminar and searching for an attractive venue.

Following the HPMPS-7 meeting in Japan, I visited Taiwan for a week at the invitation of Jennifer Kung, now an Assistant Professor of Earth Sciences at the National Cheng Kung University in Tainan. In addition to visiting NCKU, I gave a seminar at the National Research Synchrotron Science Center in Hsinchu at the invitation of Qong Cai, and participated in a Mineral Physics Special Session of the Taiwan Geosciences Assembly in Taoyuan convened by Professor Kung.

Recent activities related to NSLS II.

- On July 17, Patricia Dehmer of DOE-BES announced that the Secretary of Energy had approved CD-1 for the construction of a new synchrotron facility at the Brookhaven National Laboratory, which will be a 3.5 GeV machine called NSLS II.
- I serve on the Experimental Facilities Advisory Committee and Russell Hemley is a member of the Project Advisory Committee. Both of these com-

mittees met in May 2007 to discuss the current status of planning for this new facility. Reports of these meetings will soon be available on the NSLS website.

- On July 17-18 2007, there was a two-day Workshop for NSLS II Users. Don Weidner organized a breakout session focusing on opportunities for high-pressure research at NSLS II.

## DOE Workshop on Materials under Extreme Conditions

On June 10-12, I was an observer at a DOE Workshop on Basic Research Needs for Materials under Extreme Conditions at the invitation of Russell Hemley, one of the workshop co-conveners. I participated in the sessions on Thermomechanical Extremes co-chaired by Malcolm Nicol; Michael Brown was one of the members for this sub-panel.

## GRC on Interior of the Earth

The Gordon Research Conference on "Interior of the Earth" was held at Mount Holyoke College in Massachusetts from June 10-15, 2007, with Goran Ekstrom as Chair and Bruce Buffett as Vice Chair. More than 121 people attended, of whom 20 were from the mineral physics community. Of the 22 keynote lectures, 26% were presented by mineral physicists.

## Advisory Council of COMPRES

On Sunday, June 17, the Advisory Council of COMPRES met with the Executive Committee to discuss the current status of COMPRES and to seek the advice of the Advisory Council on strategic planning for the future, with special attention to funding initiatives.

Attending this joint meeting were:

### *Advisory Council*

Bruce Buffett  
Chi-chang Kao  
Guy Masters  
Malcolm Nicol  
Richard O'Connell

### *Executive Committee*

Harry Green  
Michael Brown

# President's Message (cont'd)

Donald Weidner  
Quentin Williams  
Mark Rivers  
Nancy Ross  
Bob Liebermann

We continue to value and appreciate the interest in and support of our organization and your sage advice from the Advisory Council as we move forward into the next five-year period of the lifetime of COMPRES.

The terms of two of the founding members of the Advisory Council ended at Lake Morey: Bruce Buffett and Rick O'Connell. We especially wish to thank them for their service during the formative years of COMPRES and hope that they will feel welcome to attend future annual meetings of our community.

Finally, we would like to welcome two new members of the Advisory Council for three-year terms commencing June 2007:

Louise Kellogg from UC Davis and  
William McDonough from the University of Maryland.

## 2007 Elections of officers and committee members of COMPRES

At the business meeting on Tuesday, June 19, 2007 at Lake Morey, Vermont, the 2007 elections were conducted. Of the 50 U. S. member institutions of COMPRES, 41 institutions voted either by mail ballot or in person at Lake Morey.

The following new officers and members of the COMPRES committees were elected.  
We congratulate all on their election.

### *Executive Committee*

Quentin Williams—Chair, 2007-2010  
Michael Brown-Vice Chair, 2007-2008; Member 2005-2008  
Carl Agee-Member, 2007-2010  
Donald Weidner-Member, 2007-2010

The other member of the Executive Committee is Jay Bass-2006-2009, as well as the Chairs of the Facilities and Infrastructure Development Committees who serve as non-voting advisors to the Executive Committee [Thomas Duffy and Nancy Ross].

### *Facilities Committee*

Thomas Duffy-Chair, 2007-2009; Member 2007-2010

He joins the other members of the Facilities Committee:

Charles Leshner-2006-2009  
William Durham-2005-2008  
Mark Rivers-2005-2008  
Wendy Panero-2006-2009

### *Infrastructure Development Committee*

Dan Shim-Member, 2007-2010

He joins the other members of the Infrastructure Development Committee

Nancy Ross-Chair [2006-2008]; Member, 2006-2009  
Pamela Burnley-Member, 2005-2008  
Russell Hemley-Member, 2005-2008  
Thomas Sharp-Member, 2006-2009

We also wish to thank the other members of the COMPRES community who agreed to stand for election:

James Tyburczy, Chair of the Executive Committee  
Jay Bass, Vice Chair of the Executive Committee  
Harry Green-Member of the Executive Committee  
Shun Karato-Member of the Executive Committee  
Charles Leshner-Chair of the Facilities Committee  
Wolfgang Sturhahn-Member of the Infrastructure Development Committee

Finally, but certainly not least in importance, we thank the following officers and committee members for their exemplary service to the COMPRES community over the past several years:

Harry Green-Chair of the Executive Committee, 2004-2007  
Mark Rivers-Chair of the Facilities Committee, 2003-2007  
Abby Kavner-Member of the Facilities Committee, 2004-2007  
Dan Shim-Member of the Infrastructure Development Committee, 2004-2007

# President's Message (cont'd)

I look forward to working with the new officers and committee members in the upcoming year to address the needs and plans of the COMPRES community.

## New Members of COMPRES

The Executive Committee has unanimously approved the applications of the following institutions for foreign affiliate membership in COMPRES:

Okayama University in Misasa, Japan, with Eiji Ito as the representative.

Universite Blaise Pascal in Clermont-Ferrand, France, with Denis Andrault as therepresentative.

This brings the number of foreign affiliate members to 30.

## Sixth Annual Meeting of COMPRES

On June 17-20, 2007, COMPRES holds its Sixth Annual Meeting at the Lake Morey Resort in Fairlee, Vermont. More than 102 professional attendees were registered and they were accompanied by another 25-30 spouses, partners and children. Details may be found in a special article in this issue of the Newsletter.

## ***Jay Bass Awarded Docteur Honoris Causa Degree***



Jay with his colleagues Bruno Reynard and Isabelle Daniel from Lyon and Carmen Sanchez-Valle from ETH in Zurich

**O**n May 25, 2007, Jay D. Bass was awarded the degree of Docteur Honoris Causa. He was cited by Isabelle Daniel and Bruno Reynard for his role in the determination of the chemical composition and of the thermal structure of the Earth's mantle from seismological data. Using Brillouin spectroscopy his laboratory has measured the varoatopm of elastic properties of numerous minerals as a function of composition, pressure and temperature. His long collaboration with the University Claude Bernard Lyon 1 has definitely nurtured the development of research in that field in Lyon, and of the work of young researchers in particular.



Jay receiving his honorary doctorate from Lionel Collet, President of the university

# 2007 COMPRES Annual Meeting Lake Morey, VT



## Sixth Annual Meeting of COMPRES

On June 17-20, 2007, COMPRES holds its Sixth Annual Meeting at the Lake Morey Resort in Fairlee, Vermont. More than 102 professional attendees were registered and they were accompanied by another 25-30 spouses, partners and children. Details may be found on the COMPRES website at:

[http://www.compres.us/Meetings/2007\\_Annual\\_Meeting/index.htm](http://www.compres.us/Meetings/2007_Annual_Meeting/index.htm)



## **Featured keynote speakers included:**

- Rob van der Hilst from MIT, “Inverse scattering of broad-band (seismic) data: New opportunities for detecting and imaging interfaces in Earth’s deep interior”
- Magali Billen from UC Davis, ‘Integrating High Pressure Experimental Constraints into Subduction Dynamic Simulations: Which ‘Unknown’ Parameters Could Have the Largest Effects?’
- Michael Hochella from Virginia Tech, “How Nanoscience Has Changed the Way We Look at the Earth”
- Francis Nimmo from UC Santa Cruz, “Moving beyond the Earth: What use is mineral physics to planetary scientists?”
- Andrea Tommasi from Universite Montpellier (France), “Linking deformation and anisotropy in the mantle”
- Malcolm Nicol from University of Nevada at Las Vegas, “Diffraction, Explosives, and Dynamics at High Pressures.”

Plus an after-banquet talk by

- Harry Green from UC Riverside, “Rocks and earthquakes from deep subduction zones: What can they tell us about water recycling, planform of mantle convection, and ocean island basalts?”

## **Additional highlights included:**

- Reports from the Community Facilities and Infrastructure Development Projects of COMPRES.
- Science posters by students and research staff.
- Breakout sessions for Graduate Students and Laser-heating DAC specialists.
- Open forum for strategic planning for COMPRES in period 2007 to 2012.

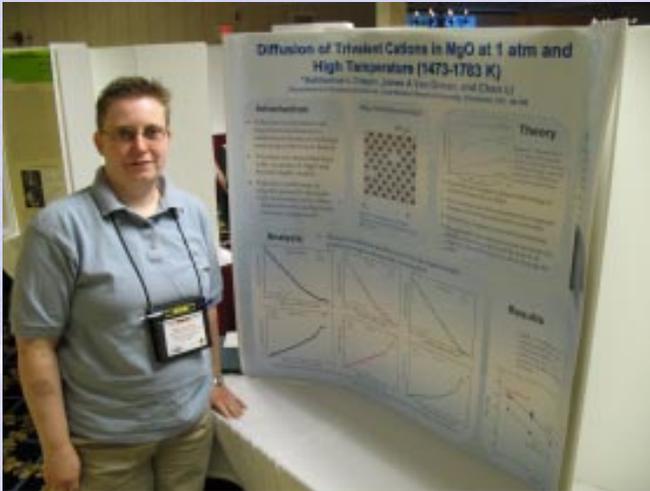
The social fund which was generously supported by the industrial sponsors made it possible to provide nice refreshments to our guests throughout the meeting; these included a welcoming reception on arrival, the poster sessions and the closing banquet.



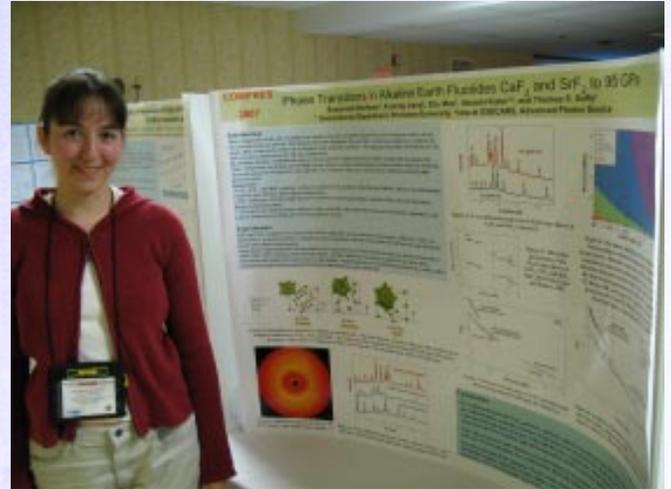
These sponsors for 2007 were:

- Almax Industries
- Blake Industries [Dave Rognlie attending]
- Bruker AXS
- D’Anvils
- Depths of the Earth
- Foxwood Instruments [Bill Bassett attending]
- Rigaku USA [George Stone attending]
- Rockland Research Corporation [Peter McNutt attending]
- Technodiamant

# Graduate Students at Lake Morey



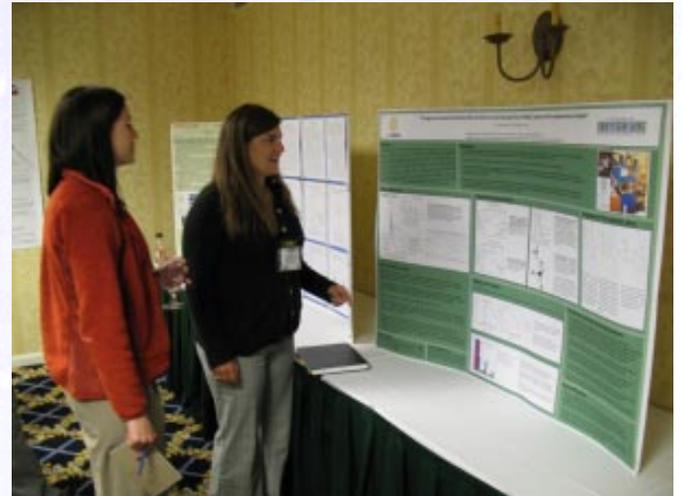
**Katherine Crispin**  
Case Western Reserve University



**Susannah Dorfman**  
Princeton University



**Lara O'Dwyer**  
University of California, Davis



**Lara O'Dwyer Brown**  
University of California, Davis



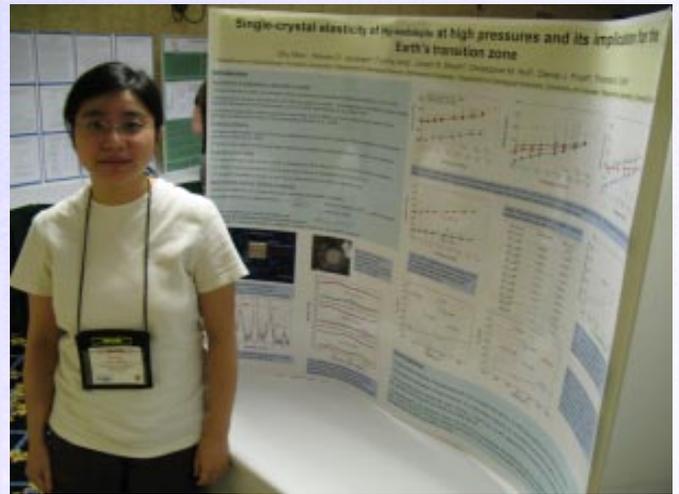
**Kimberly Kelsey**  
Stanford University



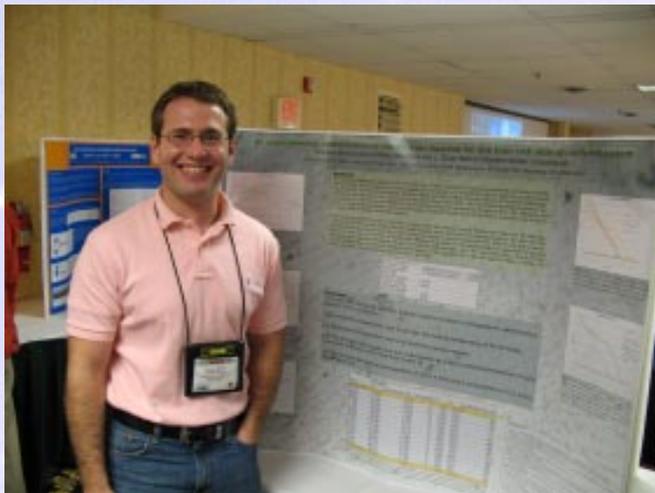
**Sabrina Huggins**  
Ohio State University



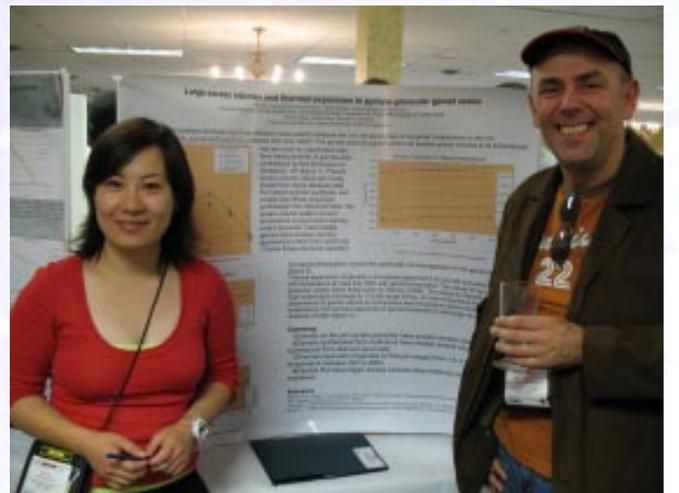
**Brent Grocholski**  
University of California, Berkeley



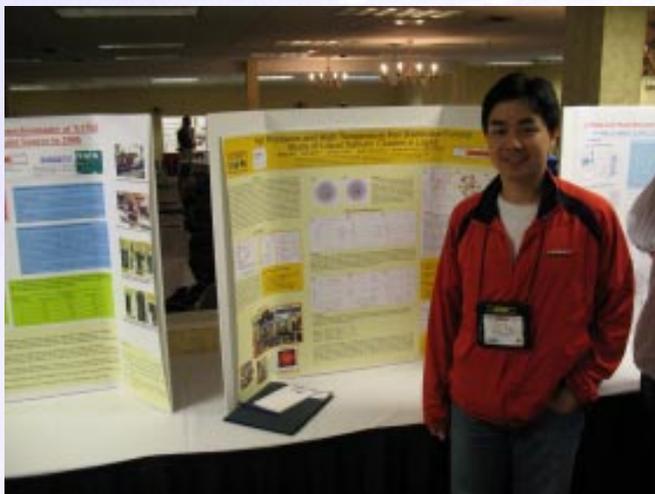
**Zhu Mao**  
Princeton University



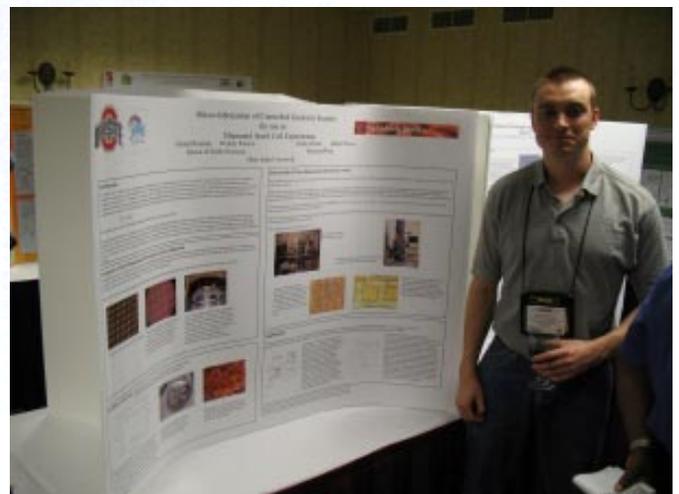
**Antonio Buono**  
Columbia University



**Wei Du**  
Columbia University



**Tony Yu**  
Stony Brook University



**Daniel Reaman**  
Ohio State University

# Recent PhDs



## *Qiong Liu*

University of Michigan, Ann Arbor -- 2005

**Equation of state for carbonate liquids and  $\text{Fe}_2\text{O}_3$ -  
and  $\text{TiO}_2$ -bearing silicate liquids**

An equation of state (P-V-T relation) for magmatic liquid is essential for calculations of equilibrium mineral-liquid phase relations at pressure, for determining the direction and velocity of magma transport in the Earth, and in a broad sense, for understanding the differentiation and evolution of the Earth and other planets.

The one-bar thermodynamic properties of the crystal and liquid are well known with the exception of the  $\text{Fe}^{3+}$  and  $\text{Ti}^{4+}$ -bearing silicate liquids owing to the composition-induced coordination change of these two cations at one bar, where it is easier to make precise density measurements than at high pressure.  $\text{Fe}^{3+}$  and  $\text{Ti}^{4+}$  provide important analogies to study the pressure-induced coordination change of  $\text{Al}^{3+}$  and  $\text{Si}^{4+}$ , which is crucial to understand the origin and processes of magma in the mantle. One-bar systematic density measurements on  $\text{Na}_2\text{O-TiO}_2\text{-SiO}_2$  (NTS),  $\text{K}_2\text{O-TiO}_2\text{-SiO}_2$  (KTS),  $\text{Na}_2\text{O-Fe}_2\text{O}_3\text{-FeO-SiO}_2$  (NFS), and  $\text{K}_2\text{O-Fe}_2\text{O}_3\text{-FeO-SiO}_2$  (KFS) liquids were conducted by double-bob Archimedean method and sound speed measurements on NTS liquids by ultrasonic interferometer. The results show that the partial molar volume, thermal expansivity, and compressibility of the  $\text{TiO}_2$  component are linearly correlated with the  $\text{Na}_2\text{O}$  and  $\text{K}_2\text{O}$  content, which are in marked contrast to what is observed for the  $\text{Fe}_2\text{O}_3$  component, where the  $\text{Fe}_2\text{O}_3$  has a compositionally independent partial molar volume and zero thermal expansivity. The results further indicate

that the  $\text{TiO}_2$  component is twice as compressible as the  $\text{Na}_2\text{O}$  and  $\text{SiO}_2$  components. In combination with the spectroscopic studies, the results show that the enhanced thermal expansivity and compressibility of  $\text{TiO}_2$  appear to be related to the abundance of the five-coordinated Ti ( $^{[5]}\text{Ti}$ ) in these liquids, but not with a change in Ti coordination. The occurrence of  $^{[5]}\text{Ti}$  in a square pyramidal site promotes different topological rearrangements in alkali titanosilicate liquids, which lead to large variations in liquid density, whereas the five-coordinated  $\text{Fe}^{3+}$  ( $^{[5]}\text{Fe}^{3+}$ ) in symmetric, trigonal bipyramidal site may not have the same topological mechanisms of expansion as the  $^{[5]}\text{Ti}$ -bearing liquids, and the relative abundance of  $^{[5]}\text{Fe}^{3+}$  may not be sensitive to the alkali content in the melt.

In addition to silicate melts, carbonate liquids attract more and more attention due to their roles in mantle metasomatism and close association with alkaline silicate magma. Furthermore, the storage of carbon in the mantle exceeds all the other reservoirs combined in the global carbon cycle. Carbonate melt may account for the anomalous seismic velocities at 280-400 km depth. Densities of carbonate liquids were determined by double-bob Archimedean method at one bar and fusion curve analysis up to 3.2 GPa. The results suggest that carbonate liquids remain strongly buoyant in the deep mantle and is highly unlikely to be a significant carbon sink in the mantle transition zone, which is consistent with the hypothesis that subducted carbonate should be reduced by Fe to diamond and stored in this form until it be reoxidized to  $\text{CO}_2$  or carbonate in lithosphere or the shallower part of the asthenosphere.

Statement:

I would like to thank my Ph.D thesis advisor Dr. Rebecca Lange and my colleagues at University of Michigan, Ann Arbor. I was exposed to and fascinated by the dynamic world of silicate and carbonate liquids, which kept me for one and a half more years' work on thermodynamic properties of ferrous iron-bearing silicate melts as a postdoctoral researcher in Michigan. I am now a postdoctoral research associate in Mineral Physics Institute at Stony Brook University working with Dr. Baosheng Li to explore the thermodynamic properties of silicate melts and metals in-situ at high temperature and high pressure by ultrasonic interferometry coupled with synchrotron X-ray diffraction techniques.

# COMPRES Sponsored Workshop



## SMEC 2007, Marco Polo Beach Resort, Miami, FL

The fourth meeting of the Study of Matter at Extreme Conditions (SMEC) co-sponsored by Florida International University's College of Engineering, the Center of the Study of Matter at Extreme Conditions (CeSMEC), COMPRES and Carnegie/Doe Alliance Center (CDAC) was held on April 16-20, 2007. The focus of the 4-day meeting was to promote interdisciplinary research in the fields of geophysics, solid state physics, high pressure physics and chemistry and materials science. The meeting brought together scholars from all over the world at the Marco Polo Beach Resort, North Miami Beach for nineteen symposia: Hydrogen Storage, Molecular systems under high compression, Structural consequences of pressure-induced electronic phase transition in iron-oxides and related minerals, High-pressure materials science: Synchrotron x-ray scattering studies, Superhard nanocrystalline materials, Chemistry and physics of the Earth's deep interior, and experiments on ferroelectrics and other active materials, Minerals at high temperature and pressure: phase

transitions, EoS and applications, The future of LVP research, Mechanical properties under extreme conditions, Earth's mantle: properties and processes, High-pressure studies of amorphous materials, liquid and melts, Laser heating of materials at high pressure, Light atoms and molecules, Extreme materials research and Miscellaneous SMEC topics. Nearly 160 scientists presented their latest research results in high pressure science at the meeting. The proceedings are to be published in the *Journal of Physics and Chemistry of Solids*. Nearly 60 papers have been submitted and currently under review. The meeting was organized by Prof. S.K Saxena with active cooperation of colleagues from GSECARS, HPCAT and several National Laboratories. A satellite meeting on Correlated Materials with Novel Function was arranged by Dr. N. Saini with 39 presentations.

COMPRES Sponsored Workshop

### COMPRES Newsletter

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